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Perspective

Multiscale energy and mass transport for a sustainable geo-energy future

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Abstract:
Multiscale energy and mass transport processes constitute the fundamental scientific foundation for sustainable geo-energy development and carbon neutrality. This perspective synthesizes cutting-edge advances in the field into three transformative thematic areas: thermodynamically consistent pore-scale modeling with robust numerical schemes that embed fundamental physical laws into mathematical formulations; molecular-scale insights and data-driven acceleration techniques bridging nanoscopic interfacial phenomena to reservoir-scale engineering; and coupled multiphysics-artificial intelligence frameworks for hydrogen infrastructure safety and supercritical CO_2 geothermal systems. Recent research reveals a paradigm shift toward living digital twins that integrate rigorous mathematical physics, multiscale computing, and artificial intelligence, charting a clear course toward carbon-neutral energy systems.

1. Introduction

Against the global imperative of energy transition and carbon neutrality, multiscale energy and mass transport processes have emerged as the critical scientific bottleneck limiting the development of unconventional geo-energy resources, gigaton-scale carbon sequestration, and next-generation geothermal systems. Subsurface energy systems exhibit inherent complexity spanning more than 10 orders of magnitude in spatial and temporal scale, with strong nonlinear couplings between thermal, hydraulic, mechanical, and chemical processes. Traditional single-scale modeling approaches, whether purely continuum-based or purely molecular, have proven inadequate to capture these cross-scale interactions. Recent advances in computational science and artificial intelligence have enabled unprecedented progress in developing integrated multiscale frameworks that preserve physical consistency while leveraging data-driven capabilities. This perspective synthesizes the latest breakthroughs in the field into three interwoven themes, identifies fundamental challenges, and outlines the emerging roadmap for future research.

2. Thermodynamically consistent and physics-preserving pore-scale modeling with robust numerical schemes

Mathematical and physical rigor is the cornerstone of trustworthy subsurface simulations (Kou et al., 2022), and significant advances have been made in developing thermodynamically consistent pore-scale models with robust numerical discretizations. Rigorous regularity analysis of two-phase flow models in porous media has demonstrated that embedding the second law of thermodynamics directly into the free-energy formulation not only restores physical fidelity but also guarantees the well-posedness of governing equations. This addresses a critical prerequisite for stable simulations under

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capillary-dominated regimes prevalent in tight reservoirs and carbon sequestration sites.

Building on this physics-driven philosophy, energy-stable finite element approximations have been developed for gas flow in poroelastic media. These fully discrete schemes are designed to inherit the thermodynamic dissipation structure at the numerical level, eliminating spurious oscillations and ensuring long-time stability essential for simulating coupled deformation and gas transport processes. For discrete pore-network modeling, a novel "flashlight algorithm" has been proposed for quasi-static drainage simulations, which efficiently tracks invading fronts through minimal-resistance percolation paths. This approach drastically reduces computational costs compared to conventional invasion percolation methods, enabling large-scale parameter sweeps that link microscopic pore structure disorder to macroscopic capillary pressure curves.

Further advances have been made in physics-preserving numerical methods for fractured porous media. An efficient enriched Petrov-Galerkin (Chen et al., 2026) method has been developed, complemented by rigorous a posteriori error estimates that enable reliable simulations in geologically complex formations. Extending thermodynamic consistency principles to non-isothermal two-phase flow, discretization strategies have been proposed that respect fundamental conservation laws at every numerical step (Chen et al., 2019). Collectively, these advances establish a new standard: the next generation of pore-scale simulators must be inherently thermodynamically consistent, algorithmically efficient, and equipped with rigorous error control mechanisms, which are no longer optional but essential for trustworthy digital rock physics and reliable upscaling to field scales.

3. Molecular insights and data-driven acceleration across scales for carbon storage and natural hydrogen

As the energy transition accelerates, understanding interfacial and transport phenomena at the molecular scale has become imperative for unlocking unconventional energy resources and enabling gigaton-scale carbon sequestration. Molecular dynamics (MD) simulations have revealed fundamental mechanisms governing natural hydrogen migration and accumulation in subsurface formations. Hydrogen molecules exhibit quantum sieving effects and preferential adsorption on clay mineral edges, fundamentally altering percolation thresholds and suggesting that naturally occurring hydrogen reservoirs may be more widespread than previously recognized.

Combined MD and Monte Carlo simulations have explored CO_2 distribution and wettability in kerogen nanopores, uncovering a profound dependence of contact angle and adsorption layering on the density and type of oxygen-containing functional groups. Organic pore surfaces can transition from CO_2-wet to water-wet under realistic reservoir conditions. This provides an insight with critical implications for assessing capillary sealing integrity in carbon storage projects. To bridge molecular understanding to engineering scales, hierarchical multiscale simulation frameworks have been developed for CO_2-enhanced oil recovery and storage, which dynamically couple MD-informed equations of state and relative permeability functions into field-scale reservoir simulators. These frameworks enable accurate prediction of complex fingering patterns and trapping efficiencies that purely continuum models fail to capture.

Addressing the computational bottleneck of molecular-scale simulations, data-driven accelerated MD algorithms leveraging graph neural networks have been developed to learn potential energy surfaces. Applied to underground gas storage in porous formations, these methods achieve orders-of-magnitude acceleration in sampling while preserving quantum mechanical accuracy, making it feasible to simulate multicomponent gas diffusion and sorption over laboratory-relevant time and length scales. The consistent message from these advances is clear: molecular-level physics is no longer an isolated academic pursuit but is being systematically upscaled through machine learning surrogates and hierarchical coupling (Liu et al., 2024), paving the way for transformative "molecule-to-reservoir" predictive workflows.

4. Multiphysics coupling and artificial intelligence-enabled systems for hydrogen infrastructure and geothermal development

At the engineering end of the spectrum, tightly coupled multiphysics simulations and artificial intelligence are addressing critical challenges in operational safety and renewable energy extraction. For hydrogen-blended natural gas pipelines, integrated frameworks have been developed that combine computational fluid dynamics for gas dispersion, structural mechanics for pipeline integrity assessment, and real-time meteorological data. These frameworks are embedded within long short-term memory neural networks that predict leakage plume evolution and provide actionable early warnings.

For subsurface energy systems, fully coupled thermo-hydraulic-mechanical-chemical models have been developed for supercritical CO_2 plume geothermal systems. These models simulate CO_2 circulation in deep aquifers, revealing that supercritical CO_2's large expansivity and low kinematic viscosity enable superior heat extraction rates compared to conventional water-based systems, while mineral dissolution effects remain manageable at realistic injection temperatures. The success of such systems hinges on accurately capturing multiscale energy and mass transport processes spanning from wellbore to reservoir scales.

These advances illustrate a broader paradigm shift: engineering-scale geo-energy systems, whether hydrogen pipelines or geothermal reservoirs, are inherently multiphysics in nature, and their safe, efficient operation increasingly depends on integrating first-principles physics models with artificial intelligence surrogates. This hybrid approach offers a practical pathway to real-time monitoring, predictive control, and optimization of complex energy infrastructures, bridging the gap between scientific understanding and industrial deployment (Creasy et al., 2024).

5. Conclusions

While remarkable progress has been made, several fundamental challenges remain that require concerted interdisciplinary effort. First, the computational complexity of fully coupled multiscale-multiphysics simulations remains prohibitive for field-scale applications. The stiff, nonlinear nature of governing partial differential equations, combined with the vast range of spatial and temporal scales involved, creates fundamental tensions between numerical stability, accuracy, and computational efficiency. Second, balancing physical consistency with data-driven flexibility presents a significant methodological challenge. There is currently no principled framework to reconcile statistical deviations from training data with mechanistic constraints, particularly under sparse or noisy field data regimes. This often leads to adversarial learning dynamics where improving physical consistency may compromise predictive accuracy, and vice versa. Third, the validation and verification of multiscale models remain problematic. As simulations span from molecular to field scales, accumulating uncertainties at each level can lead to significant discrepancies between predictions and real-world observations. Developing rigorous validation protocols that integrate experimental data across scales is essential for building trust in these models among regulators and industry stakeholders.

Looking ahead, the most promising direction is the development of living digital twins that fuse rigorous mathematical physics, multiscale computing, and artificial intelligence. Multimodal large model technologies based on Transformer architectures offer unprecedented potential to break down scale barriers through cross-modal attention mechanisms, enabling microscopic molecular insights to directly constrain macroscopic engineering simulations. However, the computational cost and data requirements of these large models present new obstacles for practical field deployment (Sun et al., 2024).

A promising future direction is to integrate physics-informed neural networks, operator learning, graph neural networks, and other advanced scientific machine-learning algorithms into multiscale geo-energy modeling frameworks (Kovachki et al., 2023). By embedding governing equations, boundary conditions, conservation laws, and thermodynamic constraints into the learning process, these methods can bridge sparse field observations and mechanistic models while supporting fast surrogate modeling, inverse parameter estimation, uncertainty quantification, and real-time data assimilation (Raissi et al., 2019). Coupled with high-fidelity numerical solvers, laboratory measurements, and field monitoring data, physics-informed artificial intelligence will be essential for developing adaptive geo-energy digital twins capable of updating uncertain parameters, quantifying operational risks, and optimizing carbon storage, hydrogen storage, and geothermal energy production strategies.

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Conflicts of interest

The authors declare no competing interest.

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